

1,4-Benzoquinone  
106-51-4 | DTXSID6020145

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.47e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 5.85e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Chlorophenol</div> <div>Measured: 9.00e-02</div> <div>Predicted: 9.27e-02</div>	<div>Image not found</div> <div>Dichlorophen</div> <div>Measured: 2.21</div> <div>Predicted: 1.12e-09</div>	<div>Image not found</div> <div>1,3-Cyclopentadiene</div> <div>Measured: 3.70e-01</div> <div>Predicted: 248</div>
<div>Image not found</div> <div>3-Bromothiophene</div> <div>Measured: 3.45e-01</div> <div>Predicted: 12.1</div>	<div>Image not found</div> <div>C.I. Disperse Red 1</div> <div>Measured: 1.17e-01</div> <div>Predicted: 1.17e-12</div>	